513.001 Molecular and Solid State Physics
3.10.2014

Problem 1

(a) The calculation of a bond potential for a molecule like N_2 is computationally intensive. Describe how this calculation would be done.

(b) Once a bond potential has been calculated, it is often fit to a Morse potential of the form,

$$U(r) = U_0 \left(\exp\left(\frac{-2(r - r_0)}{a} \right) - 2\exp\left(\frac{-(r - r_0)}{a} \right) \right).$$

It is possible to calculate the vibrational and rotational frequencies of a diatomic molecule like N_2 from the Morse potential. What are the vibrational and rotational frequencies of N_2 in terms of U_0, r_0, a, and the mass of a nitrogen atom m_N?

Problem 2

(a) Sketch approximately the phonon dispersion curves for an fcc crystal and a CsCl crystal.

(b) Define what is meant by the first Brillouin zone and explain why the phonon dispersion curves are only drawn for the first Brillouin zone.

Problem 3

In the free electron gas model for metals, there is only one parameter which can be taken to be the electron density n. (The parameter could also be taken to be the Fermi energy because for a 3D electron gas, $E_F = \frac{\hbar^2}{2m} \left(3\pi^2 n \right)^{2/3}$.)

(a) What is the density of states for a 3-D free electron gas?

(b) If you know the form of the electronic density of states and the electron density n, how could you calculate the electronic component to the specific heat?

Problem 4

The tight binding model is very similar to the method of linear combination of atomic orbitals (lcao). In both cases you contruct a trial wavefunction and calculate the energy associated with this trial wavefunction. Explain the tight binding method. What form does the trial wavefunction have? What are the differences to the method of linear combination of atomic orbitals?